Sandia RESEARCH

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COMPUTING

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Sandia National Laboratories

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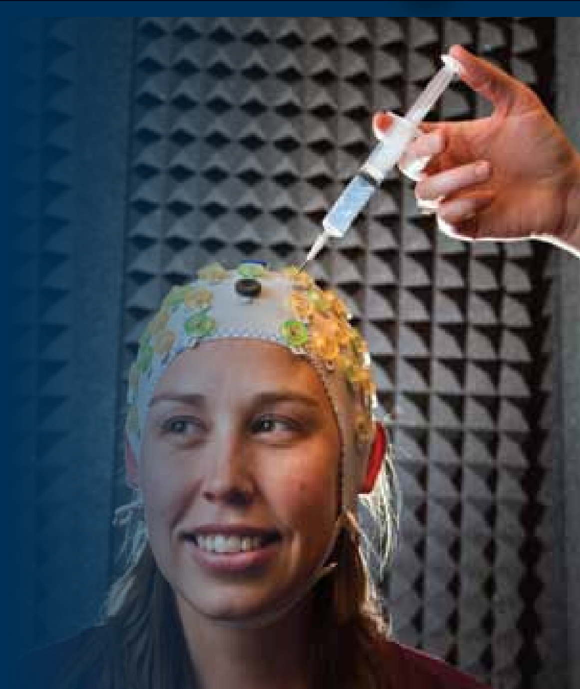
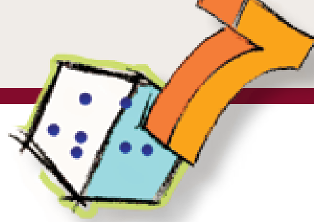
ON THE COVER

Susan Stevens-Adams wears a cap dotted with electroencephalography sensors while researchers inject them with gel to make sure each one has good contact. Cognitive systems researcher Laura Matzen used the cap on volunteers to study brain activity related to learning and memory. Matzen, who joined Sandia in 2008, studied whether signals from the brain can predict how well people will remember information they are trying to memorize. Stevens-Adams, a cognitive systems researcher at the labs, says the experience was unique and that the cap, despite how it looks, was not at all uncomfortable.

(Photo by Randy Montoya)





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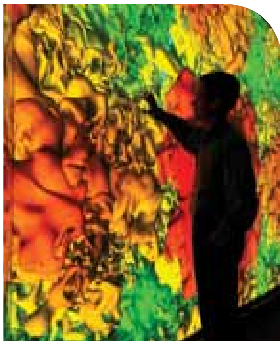

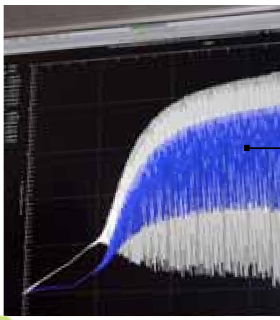

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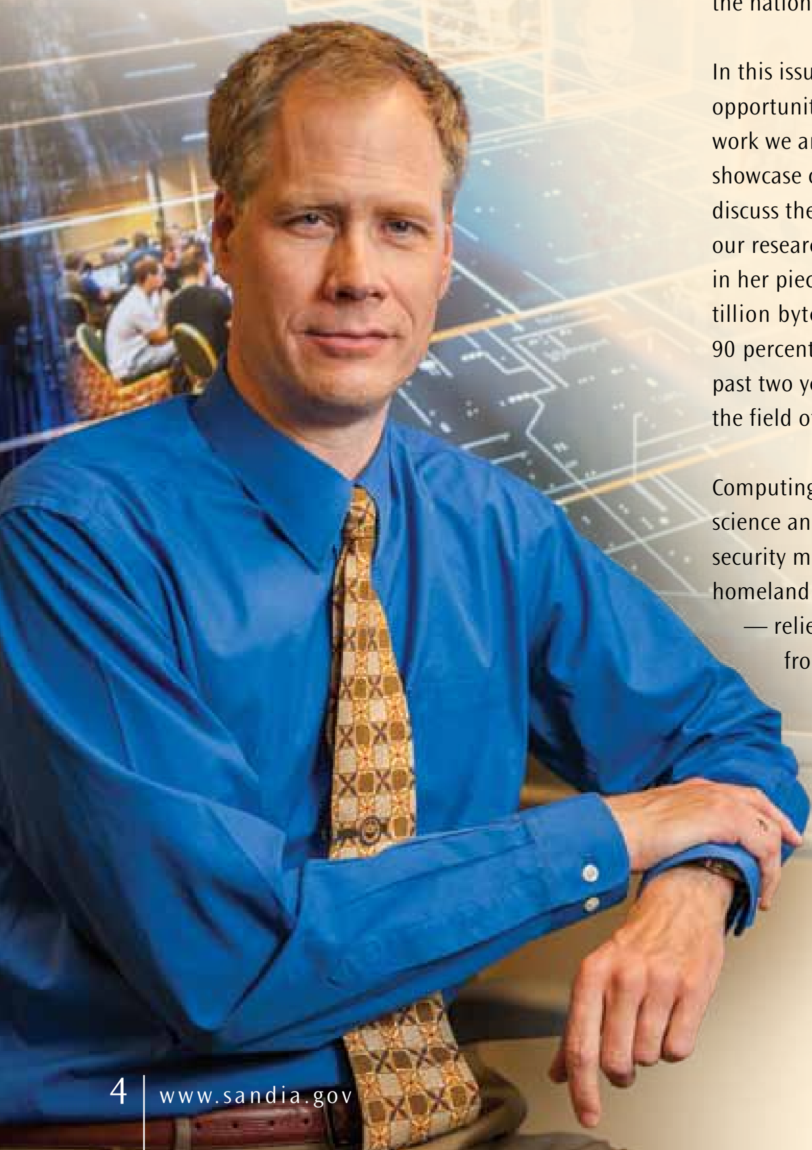
COMPUTING IS CRUCIAL
TO SCIENCE, ENGINEERING AND NATIONAL SECURITY

Advances in electronic computing technology have played a crucial role in assuring national security for six decades. Beginning with early work to discover feasible designs for the hydrogen bomb, computing has had an essential role in areas such as communications encryption, calculating ballistics tables for conventional artillery, engineering a safe, secure and reliable nuclear stockpile without underground testing, and predicting societal risks associated with weather and climate. While contributions continue in these areas, today's "needle in haystack" data analytic problems and the rapid digitalization of society into the cyber realm present unique and daunting challenges.



Much of the current national security enterprise has come to rely on the exponential increase of computer performance commonly referred to as Moore's Law. However, Moore's Law is stalling out—silicon CMOS (complementary metal oxide semiconductor) transistors are reaching their physical limits. Processor speed has already plateaued, power inefficiency is becoming a dominant concern, and within the decade circuit density will likely meet its limits. The U.S. must lead in developing next-generation computing technology in the beyond-Moore era, or face the prospect that another nation will enjoy the strategic advantages our computing capabilities have historically provided in the national security domain.

In this issue of Sandia Research, we give readers the opportunity to learn about the important cutting-edge work we are doing in the beyond-Moore arena. We also showcase our award-winning modeling code Xyce and discuss the many networking and interface problems our researchers are tackling. Patti Koning points out in her piece on tensors that according to IBM 2.5 quintillion bytes of data are created every day and that 90 percent of the data in the world was created in the past two years alone. She shows how Sandia is leading the field of interpreting large volumes of data.

Computing is ubiquitous at Sandia and is essential to science and engineering. Every one of our national security mission areas — from nuclear weapons to homeland security and defense to energy and climate — relies on advanced computing to deliver forefront solutions to our customers. Sandia's portfolio of work in this area spans fundamental research to state-of-the-art applications. We hope you find these pages informative.

Robert (Rob) W. Leland
Director
Computing and Information Sciences
Research Foundation

GET READY FOR THE COMPUTER OF THE FUTURE

New design. New materials. A whole lot better.

Computing as we know it is running out of speed.

The computer industry has operated for decades under what's dubbed Moore's Law, named for Intel co-founder Gordon Moore. He postulated in 1965 that it was economically feasible to create exponential improvement with time in the density, speed and power efficiency of integrated circuits.

By Sue Major Holmes

The idea drove a wave of technology that transformed society so that today, people carry cell phones that are little supercomputers. But the Moore's Law era — which lasted far longer than Moore himself expected — is coming to an end.

The speed of laptops and desktops has plateaued while the power required to run systems is rising sharply. And industry can't continue cramming more transistors onto chips indefinitely.

Major change is about a decade away, says Rob Leland, director of Sandia National Laboratories' Computing and Information Sciences (CIS) Research Foundation and Computing Research Center.

"We need a new type of computing device, new materials, new designs, and it's not at all clear what that should be," Leland says. "It has to be something that's not only substantially better than what we can do now, but which also can improve exponentially, because we don't want to jump to a new device technology that is also static."

The CIS Research Foundation is taking on a moon-shot goal: Develop the computers of the future.

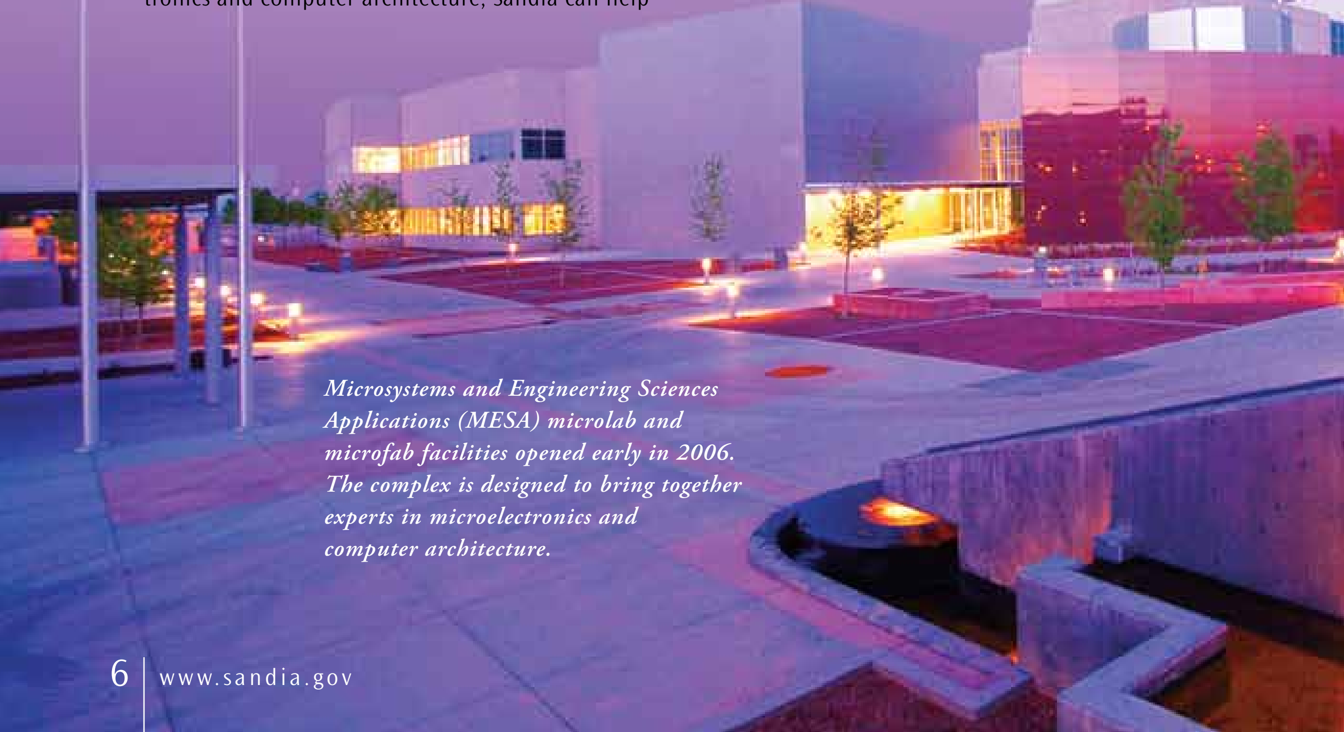
Sandia is well positioned for the challenge because of its broad supercomputer experience, from architecture to algorithms to leadership in high-performance computing.

"We think that by combining capabilities in microelectronics and computer architecture, Sandia can help initiate the jump to the next technology curve sooner and with less risk," Leland says.

Computing engineer Kathye Chavez inspects a component board in one of the many cabinets that make up Sandia's Red Sky supercomputer.

An 'epic effort'

Advances in electronic computing technology have played a crucial role in assuring national security for six decades. This began with early work to discover feasible designs for the hydrogen bomb, exploit encryption, calculate ballistics tables for conventional artillery and predict risks to society associated with weather and climate. The effort continues today with work to engineer a safe, secure and reliable nuclear stockpile and to solve "needle in haystack" data analytic problems.



Microsystems and Engineering Sciences Applications (MESA) microlab and microfab facilities opened early in 2006. The complex is designed to bring together experts in microelectronics and computer architecture.

The plateauing of Moore's Law is driving the energy costs of modern scientific computers ever higher, to the point that if current trends hold, future supercomputers would become impractical due to their enormous energy consumption. Leland says resolving the challenge will require new computer architecture that reduces energy costs, which are principally associated with patterns of moving data within the system and thus can be improved. And eventually, it will require new technology at the transistor device level that uses less energy.

Sandia can make important contributions in the physics and architecture of future computing and in components “that would be assembled into a new system that would require a new software ecosystem, and that would require new approaches to applications,” Leland says. “So essentially the whole stack, the whole set of technologies that layer on top of one another, will have to be redone to some degree, perhaps radically in some cases.”

And with scientific, manufacturing and economic hurdles to work through, “it’ll be an epic effort,” he says.

Sandia won’t develop the next generation alone but can play a key role because of its leadership in computer architecture and thanks to MESA, the Microsystems and Engineering Sciences Applications complex, which does multidisciplinary microsystems R&D and fabricates chips to test ideas.

“It doesn’t really help us if we have a new device that we then can’t engineer into a system,” Leland says. “It’s really the combination of the microelectronics capability, the computer architecture capability and all the different layers that come with that. For example, that would require new operating systems, new tools and algorithms, and so on.”

MESA integrates disciplines throughout the Labs. It can invent, test and scale new information technologies and is at the heart of Sandia’s work on exascale, quantum and other emerging technologies post Moore’s Law, says Gil Herrera, director of Microsystems Science, Technology and Components, who runs MESA. Exascale computing aims to achieve a billion billion operations a second without excessive energy use, while quantum technology seeks to find ways

to use the interaction of atoms and particles to process information in new and highly efficient ways.

"At MESA, we can explore beyond-Moore technologies using approaches that are scalable to high-volume manufacturing," Herrera says. "MESA is a magnet that attracts researchers from across Sandia, from universities and industry interested in meeting the challenges posed by the end of Moore's Law. We have the flexibility to investigate different materials, devices, architectures and concepts."

Different systems for different tasks

Sandia, in response to a call from the U.S. Department of Energy for ideas for major new experimental science facilities, has proposed a Center for Heterogeneous Processing and Packaging, or CHIP^2, an acronym meant to invoke a computer chip. The center would advance microsystems research, particularly for the nuclear weapons program; expand cybersecurity efforts in providing trusted microelectronics; and increase computing research and development. Leland says the center is 10 to 15 years away, but would keep DOE at the forefront of technology and attract a new generation of talent.

As a national laboratory, Sandia is able to take an independent, critical look at how proposed future technologies work, when they might be feasible and what risks each entails, says Erik DeBenedictis, who works in the Advanced Device Technologies Department. He also credited Sandia's unique position to strong electronics research built on its nuclear mission and to MESA.

"We have a fab that allows us to actually experiment with these devices by making them and seeing how well they work. … We can explore the designs, we can explore the materials, we can explore the architectures and the function. And if they look good, we can transfer the technology to industry," he says.

The integrated circuit technology behind today's computing is called CMOS, for complementary metal oxide semiconductor. CMOS still

MEET

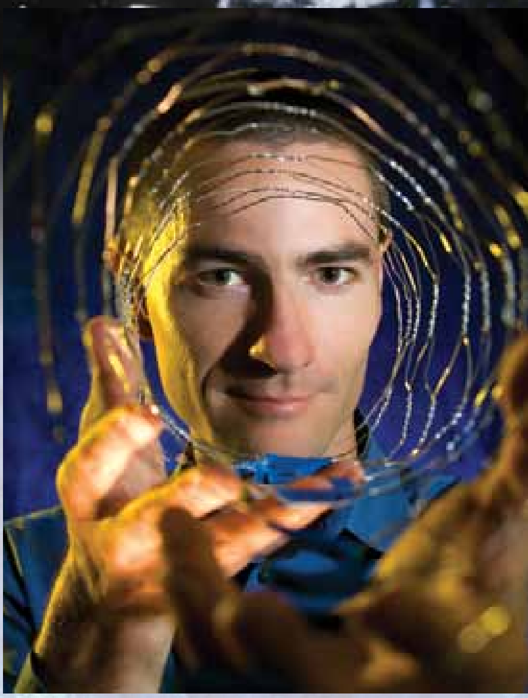
Erik DeBenedictis

DeBenedictis joined Sandia after his startup company failed. His first day of work was Sept. 10, 2001 — the day before 9/11. "I came to Sandia to earn a living after suffering a setback. I had no idea that on my second day on the job, national security work would experience a big boost."

STATS

- Bachelor of science in electrical engineering from Caltech
- Master of science in electrical engineering (computer engineering) from Carnegie Mellon
- Ph.D. in computer science from Caltech

- Works for Sandia's Advanced Device Technologies Department.
- As a grad student and post doc at Caltech, DeBenedictis worked on the hardware that turned into the first hypercube multiprocessor computer. Later dubbed the "Cosmic Cube," it ran for more than a decade after he left the university and was copied over and over. It's considered the ancestor of most of today's supercomputers.
- In the 1980s, DeBenedictis, then working for Bell Labs in Holmdel, N.J., was part of a consortium competing for the first Gordon Bell award. The award, which recognizes outstanding achievement in high-performance computing, ultimately went to a team from Sandia.



Above, physicist Mark Boslough describes the simulated destruction of an asteroid. His research is an example of the high-impact scientific work done through the integration of Sandia-designed supercomputing hardware and sophisticated applications codes. Left, physicist François Léonard holds a wire mesh cylinder similar in design to a carbon nanotube that might form the basis for future computing technology.

goes by that name, even though in the evolution of the technology oxygen was replaced about a decade ago by hafnium.

Various technologies beyond CMOS may be on the horizon, including tunnel FETs (or field effect transistors, in which the output current is controlled by a variable electric field), carbon nanotubes and superconductors, as well as entirely new approaches such as quantum computing and artificial neural network systems, also called brain-inspired computing. Sandia works in all those areas, and the future of the Information Age may be one of different systems for different tasks, DeBenedictis says. FETS, carbon nanotubes and superconductors could make exascale computing feasible at dramatically lower power levels. Quantum computing and brain-inspired computing go beyond the exascale.

Tunnel FETs and carbon nanotubes are changing the structure of transistors in ways Moore could not have realized when he made his prediction, DeBenedictis says. Exotic superconductors, which run at liquid helium temperatures, would cut energy use and could transform future large data centers, while quantum computing is good for special problems but would be tremendously expensive for general-purpose computing. A brain-inspired computer learns, and while that's of interest to the industry, it won't run existing codes faster. It might run new codes or enable new applications, but that won't address the market for computers to run such things as Facebook server code faster, DeBenedictis says.

"I think where we're going is that classic tunnel FETS and beyond-CMOS transistors could continue Moore's Law for general computing, including cell phones; superconductors are probably limited to data centers; brain-inspired computers are limited to new apps; quantum computing looks pretty special. … It's not just one system anymore," he says. ■

XYCE

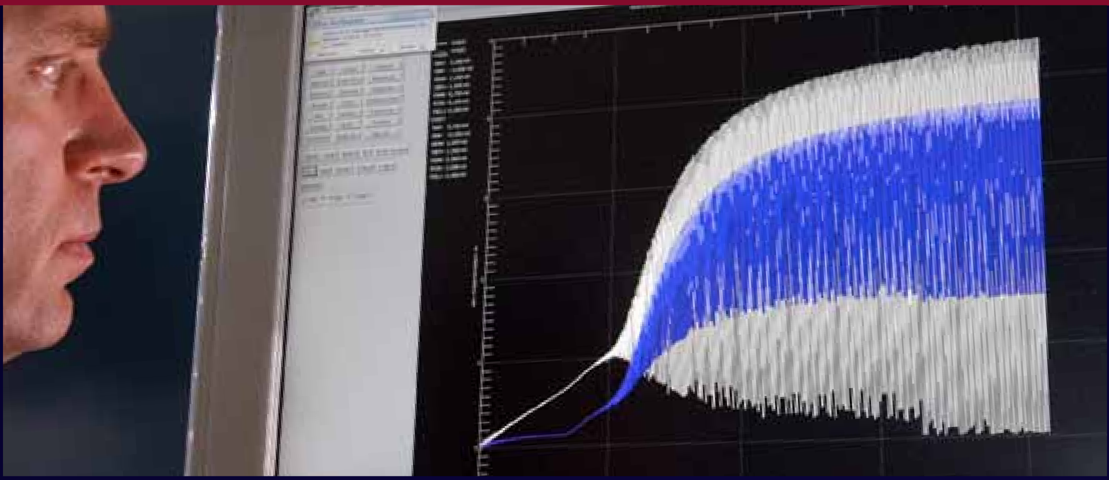
(rhymes with nice)

A modeling code could one day unlock the secret to computer systems that learn, adapt and deduce — like a brain

By Sue Major Holmes

A map of electronic circuitry looks a lot like a map of the brain. That's led Sandia researchers to apply a computing code to research into those excitable cells called neurons and even the futuristic idea of brain-inspired computing.

Sandia started developing the code called Xyce (pronounced Zys) in 1999. Designed for modeling large-scale circuits, Xyce has been used to simulate electrical circuits and neuron systems and was studied for use in simulating power grids as it matured, says Eric Keiter, principal investigator on the Xyce project. In 2008, Xyce received an R&D 100 award, one of the so-called "Oscars of Innovation."



Scott Hutchinson studies a computer simulation of a voltage waveform from an oscillator circuit. Such simulations take good advantage of Sandia's home-grown XYCE software.

A core use at Sandia is modeling circuits in a radiation environment. Xyce is different from other circuit simulators because it includes the physics needed to model radiation effects and distinctive mathematics for solving large-scale circuit problems.

To modelers, a circuit is just a network that connects devices whose behavior is governed by differential algebraic equations, in contrast to other types of simulators that solve problems governed by partial differential equations, says Scott Hutchinson, who manages Sandia's Electrical Systems Modeling Department.

That uniqueness makes Xyce applicable to such complicated problems as neural simulation.

Projects at Sandia have increasingly turned to Xyce for complex modeling. A Laboratory Directed Research and Development (LDRD) project four years ago that wanted to measure neuron activity in laboratory cultures tapped Xyce for more detailed modeling than possible with programs used by the neuroscience community, says Richard Schiek, who also works in electrical systems modeling.

Xyce successfully performed small-scale modeling for the complicated computational neuroscience project. The question for a follow-up LDRD project was this: If Xyce could model such complex nonlinear circuits, could researchers extend the high-fidelity simulations of neuron systems to build a model that would replicate a system of neuron synapses interacting with one another?

Traditionally, simulating neurons has meant simplifying what a neuron looks like. But Schiek says Xyce can implement a more detailed model, "and that model looks like a circuit when you write out all the equations and connections." Unlike a simple model in which each neuron is a single point in the simulation, Xyce better represents reality, in which neurons are large branched structures connected to neighboring neurons.

"...simulating neurons has meant simplifying what a neuron looks like."

"On average, the neurons in your brain are connected to from one thousand to 10 thousand other neurons, whereas in a circuit most devices are connected only to a few other devices near them," Schiek says. Still, the follow-up LDRD discovered much of the work that went into Xyce translated well to solving more complex connectivity problems. Next up for neuroscientists is learning how to model realistic behavior in collections of neurons.

In another arena, there's the idea of building an electrical circuit on circuit components or devices that behave like neurons and synapses. The goal would be a future-generation computer inspired by how biology works — brain-inspired computing. In a traditional circuit, components or devices are resistors or capacitors, while in a neuron circuit they're neurons and synapses.

The brain is an efficient computer for such things as pattern recognition, able to operate with high connectivity and low power. Although brain-inspired computing is in the very early stages of exploration, it's attractive because the potential payoff in efficiency could be enormous.

About 40 years ago, a Berkeley professor proposed a hypothetical device called a memristor, Keiter says. Hypothesis became reality about five years ago when industry figured out how to make such a device, which behaves more like neurons and synapses than normal computer circuitry, he says.

The idea behind a memristor is that if a circuit pathway is used a lot, resistance is low and it's easy for it to make a connection, whereas if it's not used often, resistance would be high and imply the two units are not working together.

Since Xyce simulates electrical domain problems, "can you start to incorporate models for new devices like memristors and assemble a system that can do something useful like pattern recognition? And can you use that as a way to design a more complicated system?" Schiek asks.

The connection to brain-inspired computing is the comparison to synapses, he says. When two neurons near each other frequently communicate, their synapse becomes very active. The more active, the easier it is to translate the activity in one neuron to the other.

Such high connectivity is characteristic of neuron structures, giving researchers an opportunity to figure out ways to take advantage of it while minimizing the communication costs that rise as connectivity increases, Hutchinson says.

"The most complicated, most powerful computers we build now basically take a power plant to run. They're huge," he says. "And yet they're not anywhere nearly as complex or as powerful as the brain. The brain runs on the power of a light bulb, roughly. So there are immense efficiencies in how the brain computes that we're not even close to realizing in our state of the art for computing technologies." ■

MEET

Richard Schiek

Schiek has enjoyed amateur astronomy most of his life. "When it's dark and the sky is clear, I love to head outside with a pair of binoculars or a telescope and look for star clusters, nebula, double stars and planets. When I got a job offer from Sandia I was thrilled because I would get to live in a state with really great, clear dark skies — at least when it's not the monsoon season — and at the time I was living in the Netherlands where it rains a great deal. Looking up at the sky is amazing in that one can take in the expansive universe and how fortunate we are to live on, as Carl Sagan put it, this 'pale blue dot.'"

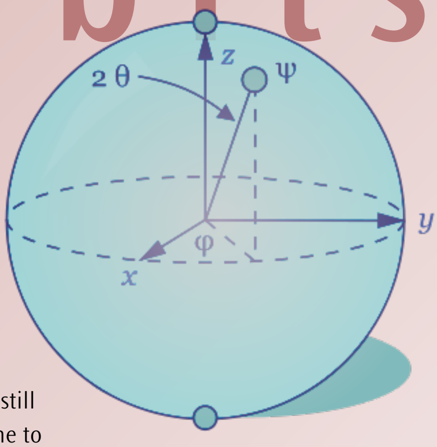
STATS

- Bachelor of science in chemical engineering from the University of Illinois at Urbana
- Master of science and Ph.D. in chemical engineering from Stanford University. He jokes that Stanford's full name is the Leland Stanford Junior University, "so technically I got my degrees from a 'junior' university."
- As an undergraduate, Schiek wrote computer code to help psychologists analyze data from a study on how social support networks help make people more resilient in difficult times.
- He later worked with a nonprofit group that helped keep people from becoming homeless. He said it was rewarding to move from theory to practice, and keep the technical work of graduate school in perspective.

what's next

High Noon for qubits

By Neal Singer



In the twilight of Moore's Law, researchers around the world are searching for efficient, reliable quantum bits, or qubits, to replace ordinary bits, the little yes-no circuits that are the bread and butter of today's computers. Exceptional qubits would be vital to a far faster, more energy-efficient quantum computer.

"There are a half dozen methods that might achieve working qubits," says Sandia Advanced Device Technologies manager John Aidun. "It's still the Wild West out there, and fun, as long as you can convince someone to pursue the work."

Computational modeler Rick Muller threw his hat in the ring, using quantum double dots and embedded donor atoms to create qubits with help from Sandia's Microsystems and Engineering Sciences Applications complex and Ion Beam Laboratory and the Center for Integrated Nanotechnologies, a Department of Energy facility jointly operated by Sandia and Los Alamos national laboratories.

Quantum dots are nanoparticles of semiconductor material. Donor atoms add electrons. Together they create small "puddles" of electrons in a semiconductor system. And they require only standard microelectronic fabrication techniques.

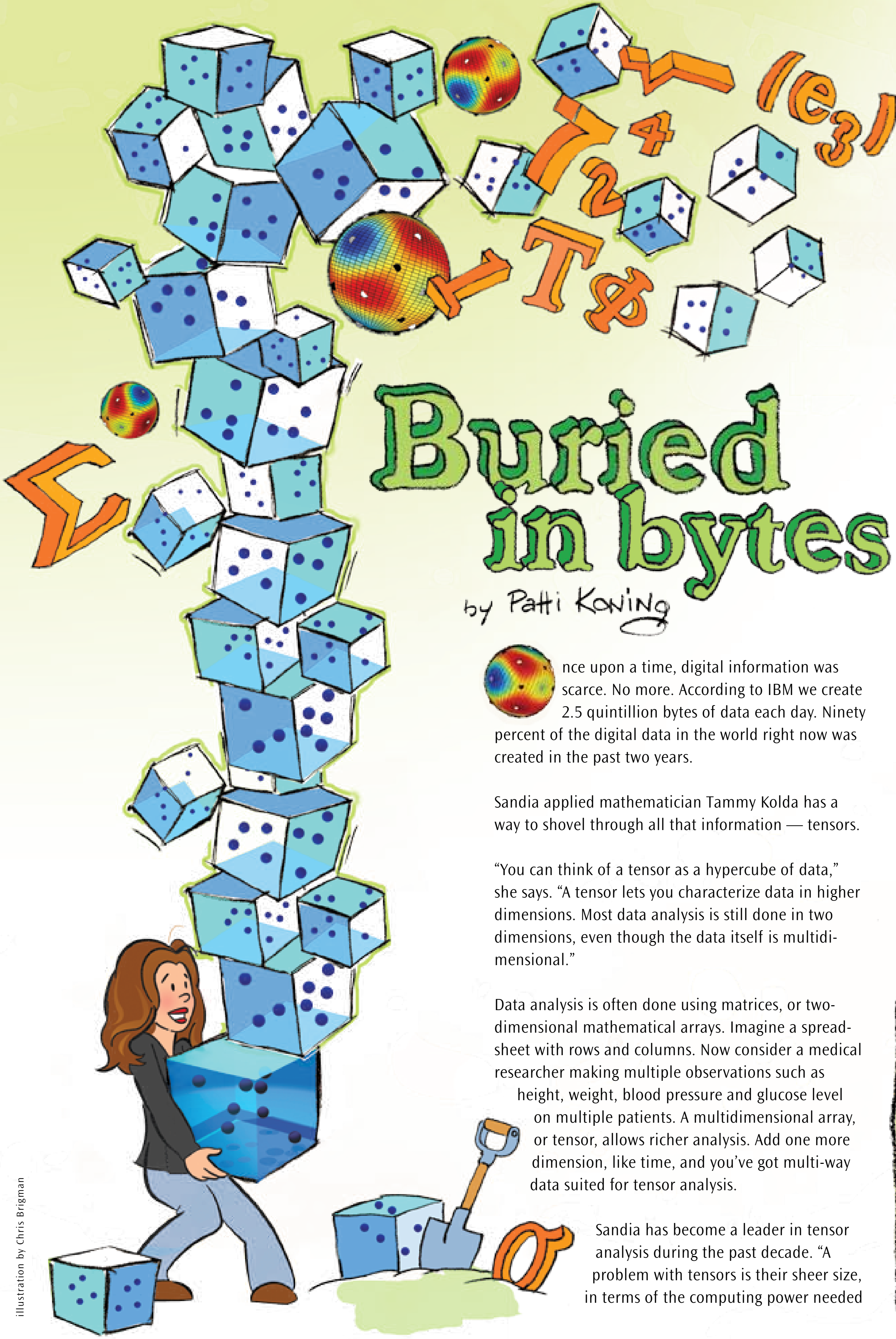
Muller colleagues Erik Nielsen, Ralph Young and Xujiao (Suzey) Gao write software to accelerate development of the donor and dot devices. Their Quantum Computer Aided Design (QCAD) software can predict properties of qubit structures before they are created in the laboratory and help identify promising candidates among various designs. The modelers work closely with experimental scientists to ensure the software becomes a valuable tool for the research team.

The semiconductor qubits use the electron's spin to deliver information. Because the spin's direction is either up or down relative to an external magnetic field, the natural two-level systems can define a quantum bit. And because of the exotic properties of quantum mechanics, electron spins can be in a "superposition" that lets them spin up and down at the same time. Classical bits are either on or off but not both. A computer made from qubits can use that difference to solve some thorny computational problems more efficiently.

The joint efforts of the modelers and the experimental groups are paying off. Experiments have identified donor systems with long decoherence times — up spins change slowly to down spins — suggesting there will be enough time to run computations before the qubit fully decoheres. ■

A quantum bit is the fundamental unit of quantum information. But unlike classical bits, which store information in either a "0" or a "1" state, quantum bits can take on values between "0"and "1," inclusive.

Because of special properties not found in the realm of classical physics, quantum-bit-based computing could greatly speed up processing. It also could help solve problems that are extremely challenging for today's computers.



Buried in bytes

by Patti Koning

Once upon a time, digital information was scarce. No more. According to IBM we create 2.5 quintillion bytes of data each day. Ninety percent of the digital data in the world right now was created in the past two years.

Sandia applied mathematician Tammy Kolda has a way to shovel through all that information — tensors.

“You can think of a tensor as a hypercube of data,” she says. “A tensor lets you characterize data in higher dimensions. Most data analysis is still done in two dimensions, even though the data itself is multidimensional.”

Data analysis is often done using matrices, or two-dimensional mathematical arrays. Imagine a spreadsheet with rows and columns. Now consider a medical researcher making multiple observations such as height, weight, blood pressure and glucose level on multiple patients. A multidimensional array, or tensor, allows richer analysis. Add one more dimension, like time, and you’ve got multi-way data suited for tensor analysis.

Sandia has become a leader in tensor analysis during the past decade. “A problem with tensors is their sheer size, in terms of the computing power needed

illustration by Chris Brigman

to work with them," Kolda says. "You aren't going to store a dense 10,000 by 10,000 by 10,000 tensor on a standard computer."

While the blocks of data are huge, there isn't always a lot of data inside. For example, in analyzing transactional data like email traffic, many entries will be zero. "If you look at a group of people, only a few pairs are emailing each other in any given time period," Kolda says. "We don't have to store those zero entries. Instead, we store a sparse tensor that is smaller and easier to analyze."

Sandia is the primary source of sparse-tensor software, developed with two Laboratory Directed Research and Development projects and an investment from the U.S. Department of Energy Office of Science that recently was renewed for another three years.

As big data gets bigger, a mathematician looks at digging out with multi-dimensional storage cubes. Her work could revolutionize computing as we know it.

"Tensors are applicable almost everywhere," Kolda says. "If you have big data, tensor decompositions can yield deep insights." Tensor decomposition is a mathematical procedure that converts multidimensional data into sets of correlated observations and is frequently used in exploratory data analysis.

Breakthroughs in medical technology are a major source of big data. Kolda is working with several universities on diffusion tensor imaging (DTI), an advanced magnetic-resonance imaging technique that maps the diffusion process of molecules in biological tissues and distinguishes gray matter from white matter. It is particularly important to neurosurgeons who need to avoid white matter.

"The analysis requires a tensor factorization for every single voxel [the 3-D equivalent of a pixel] of data, so we're talking millions of calculations. You quickly hit a wall with the sheer size of the data," Kolda says. Her group is developing symmetric tensor algorithms that quickly interpret the data. The ultimate goal is real-time imaging during surgeries.

No ordinary toolbox

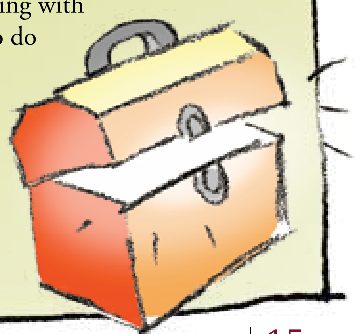
Tammy Kolda and other pioneers in the field of sparse tensors had to invent their own tools, most notably the Tensor Toolbox for MATLAB.

"About eight years ago my group was working on a project to apply tensor analysis to graph data, but the data was too big to store as a tensor," she says. "We made our own data structure to solve this problem, which is now being used by thousands of people worldwide."

MATLAB is a high-level language and interactive environment that lets users perform computationally intensive tasks faster than with traditional programming languages. The Tensor Toolbox is a collection of six object-oriented classes for efficient numerical calculations with large-scale multidimensional arrays. Users can quickly devise prototype advanced algorithms.

"The Tensor Toolbox makes working with tensors as easy as MATLAB makes working with matrices," Kolda says. "The user doesn't have to worry about the low-level details to do complex, high-level operations."

The Tensor Toolbox is most commonly used for data mining, but there are other applications that have surprised Kolda, such as watermarking, music genre classification, air traffic control, continuum mechanics and quantum entanglement. And students are even downloading the Tensor Toolbox to complete homework assignments.



Tensors also may be key to reducing communications in standard computational kernels, the main component of a computer's operating system. Gray Ballard, who worked with Kolda for two summers as a graduate student at the University of California, Berkeley, will return to Sandia this fall as a Truman Fellow to tackle the problem.

Ballard worked on tensors, but he and Kolda also spent time talking about his research in communication-avoiding algorithms. "Moving data on a computer has a big cost in terms of both time and energy. Finding ways to avoid moving data reduces the expense and time for calculations," Kolda says.

To see how this relates to tensors, you have to go back to 1969 when Volker Strassen developed a new method for matrix multiplication that reduces both computation and communication costs. "Tensor factorizations hold the key to improving on Strassen's method by expressing matrix multiplication as a tensor and then decomposing it," Kolda says.

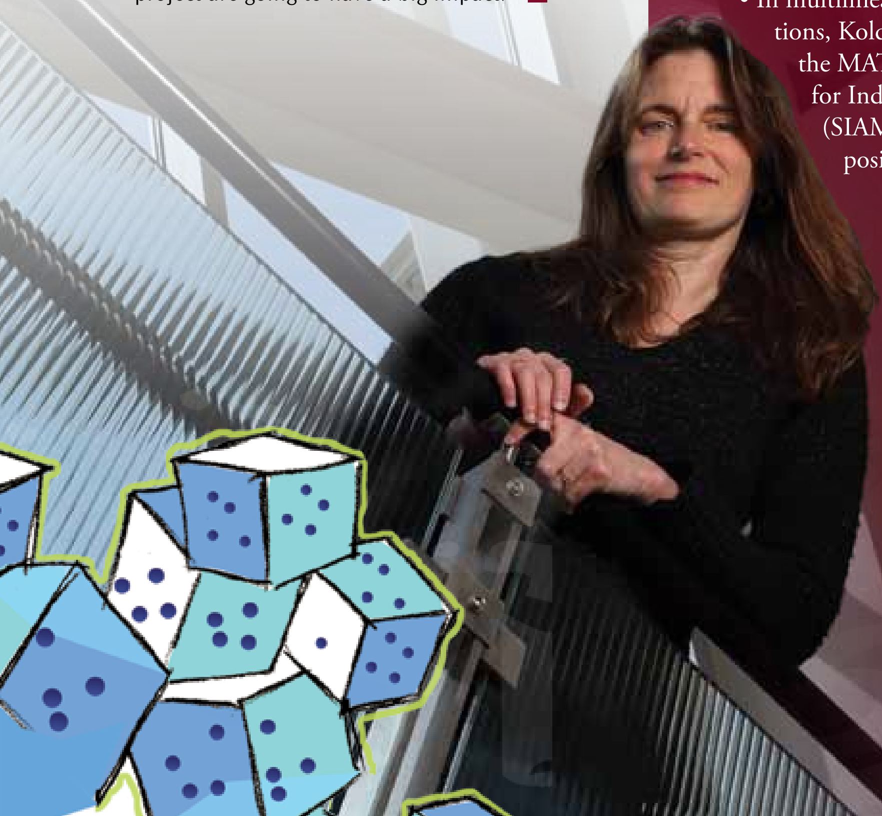
"It's kind of crazy that this 50-year-old math concept can be expressed as a tensor decomposition. It's also really exciting, because we can apply our knowledge of tensor decomposition to a problem that could revolutionize computing as we know it. Even the incremental gains we make in this project are going to have a big impact." ■

MEET Tammy Kolda

Kolda teaches a weekly flow yoga class at Sandia. She began practicing yoga 12 years ago as a new exercise challenge. "To me yoga is much more interesting and challenging than other exercise classes. There is a lot of emphasis on form and breath. Yoga is endlessly deep. Whenever you think you have mastered something, there is always more to learn," she says.

STATS

- Bachelor of science in mathematics from University of Maryland, Baltimore County
- Master of science and Ph.D. in applied mathematics from University of Maryland, College Park
- Householder Postdoctoral Fellow in Scientific Computing, Oak Ridge National Laboratory
- Joined Sandia in 1999 and works in the Informatics and Systems Assessments group.
- Kolda's current research interests include network modeling and analysis, multilinear algebra and tensor decompositions and compressed sensing.
- In multilinear algebra and tensor decompositions, Kolda is best known for her work on the MATLAB Tensor Toolbox and a Society for Industrial and Applied Mathematics (SIAM) Review article on tensor decompositions and applications.
- Kolda is a Distinguished Member of the Association for Computing Machinery, an elected member of the SIAM Board of Trustees, section editor for the Software and High Performance Computing section of the SIAM Journal on Scientific Computing and an associate editor for the SIAM Journal on Matrix Analysis.



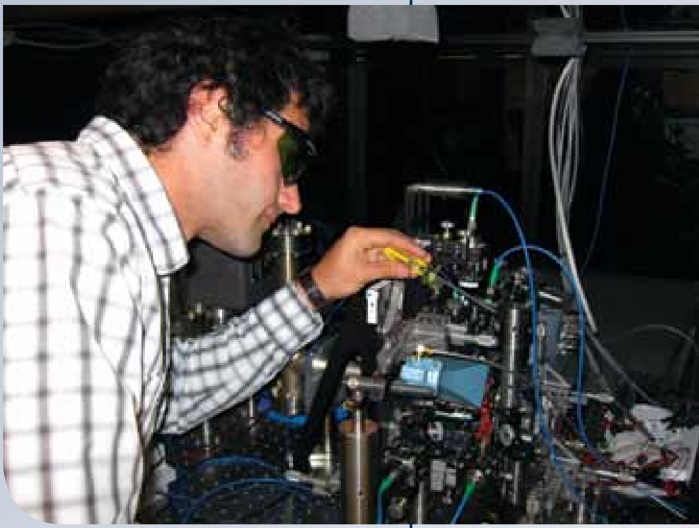
what's next

Through a quantum tunnel

By Neal Singer and Toby Jacobson

Quantum computing has captured the imagination of researchers because it promises to solve problems that overwhelm a classical computer.

But quantum computation relies on the delicate handling of quantum bits, or qubits. Among the technologies researchers are experimenting with are trapped ions, electrons in semiconductors and magnetic flux in superconductors. These require isolating qubits from the environment while allowing the operator to control and manipulate them.

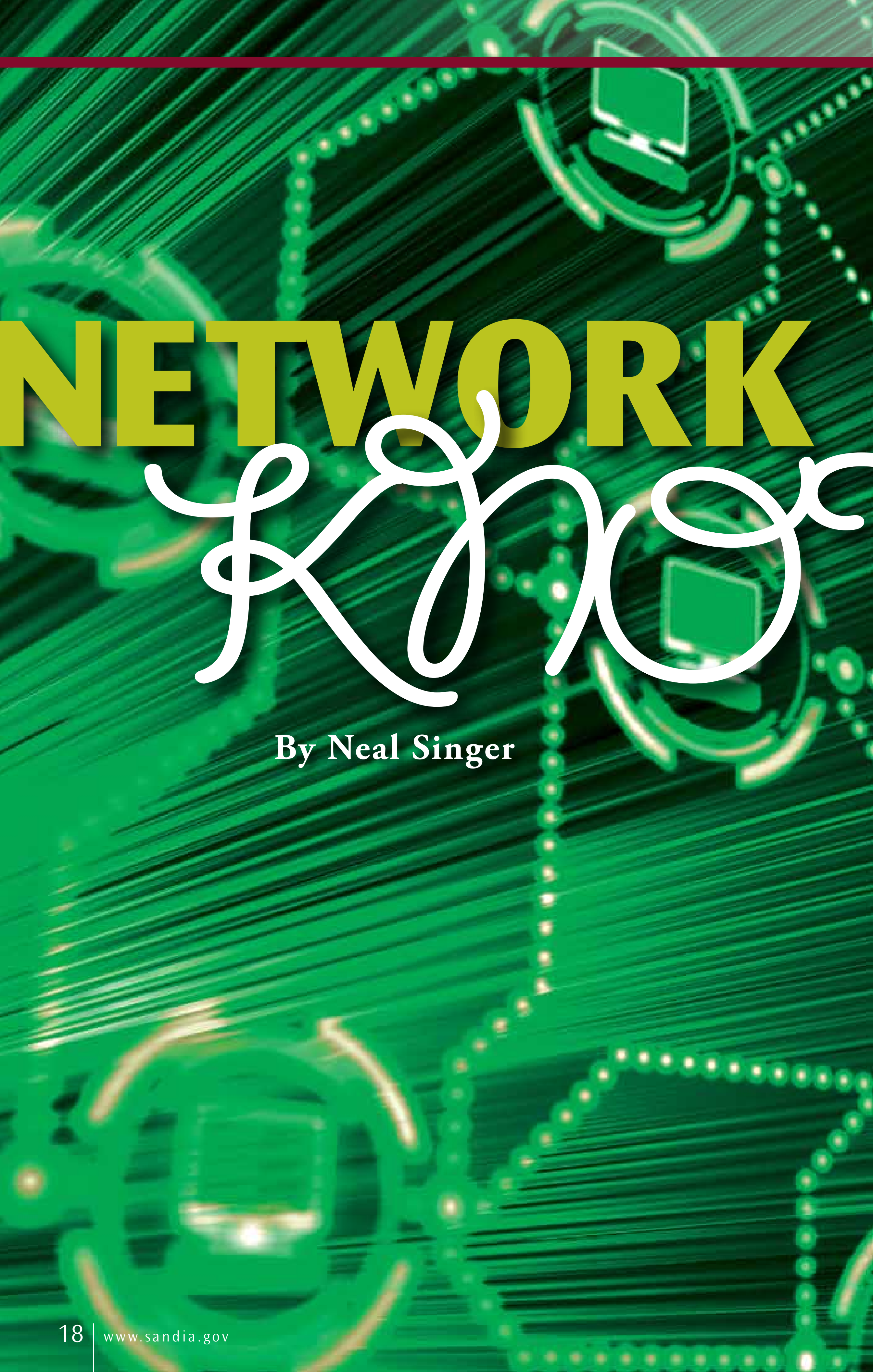


Researcher L. Paul Parazzoli adjusts Sandia's first operational (one-qubit) quantum processor. Because these superposed states of one qubit can be combined with other superposed qubits, a string of quantum bits has an enormous capacity for encoding information.

Achieving a balance between isolation and control is a daunting challenge. Sandia's AQUARIUS project explores an alternative design for a quantum computer that could provide greater immunity to environmental noise. Called adiabatic quantum computing (AQC), it expresses the solution to a problem as the lowest energy configuration, or ground state, of the collection of qubits in the computer. The ground state is obtained by exploiting the phenomenon of quantum tunneling to transform an initial, easily produced configuration of qubits into the complex configuration that gives the solution.

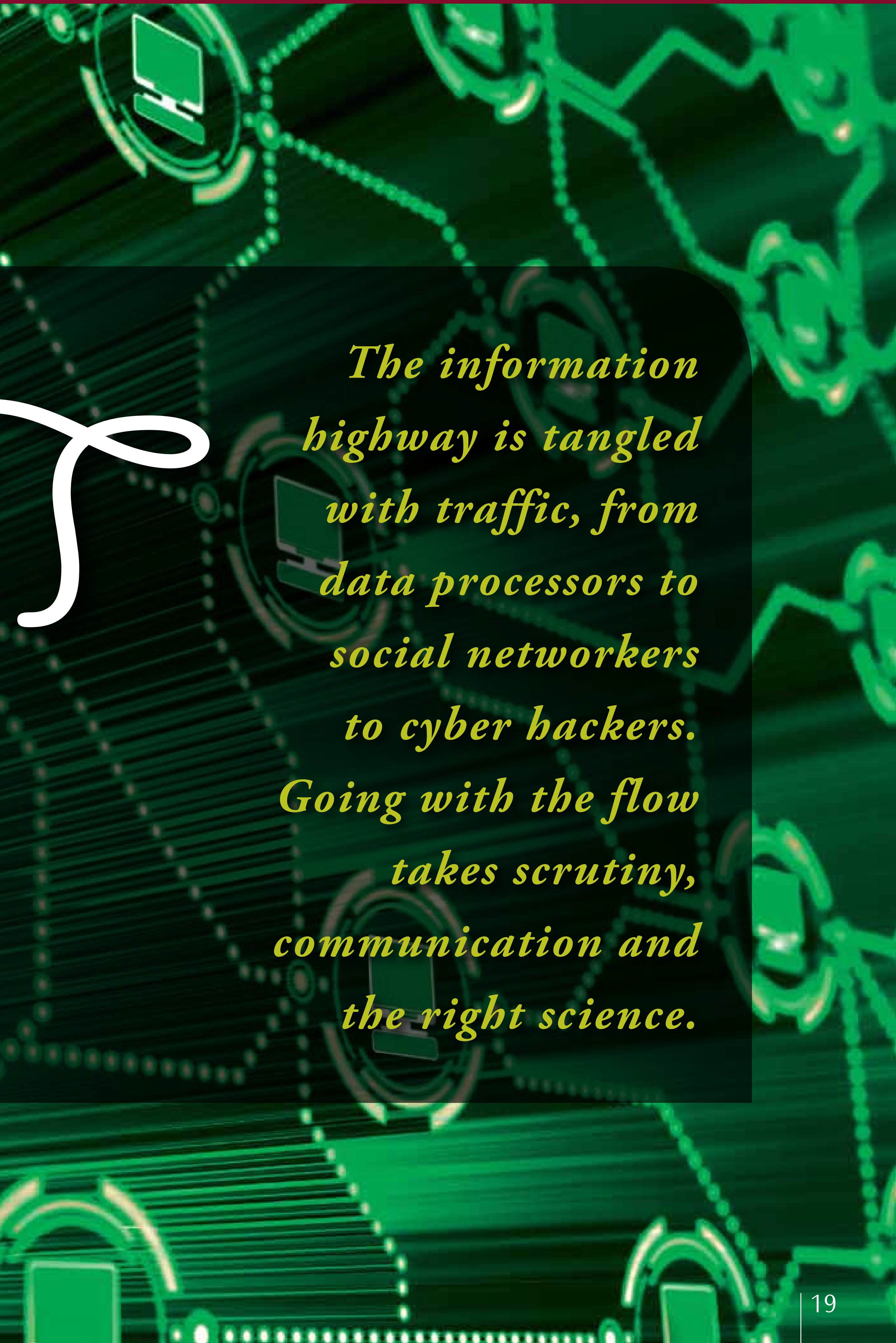
Cooling the qubits eventually leads to the ground state, but can take a long time. Quantum tunneling can bring about the ground state dramatically faster for some problems. But how to verify that the ground state was a result of quantum tunneling rather than thermal cooling? AQUARIUS started with a single qubit and developed a test that answers the question.

The test identifies whether quantum tunneling has taken place. As scientists build more advanced devices for adiabatic quantum computation, it is critical to test and establish their quantum nature at each stage of development. Preserving the delicate properties of a quantum computer makes the quantum speed-up over classical computers possible. ■



NETWORK kno

By Neal Singer



The information highway is tangled with traffic, from data processors to social networkers to cyber hackers. Going with the flow takes scrutiny, communication and the right science.

In the beginning there was Superman, and he flew alone. Batman and the Green Hornet had helpful squires. Today's superheroes network: The Fantastic Four combine their skills to battle evil.

Networking is even more pronounced in computing. It is no longer the lone eagle but networks that do the heavy lifting in preventing sabotage or piecing together large amounts of data, say Sandia computer experts.

In national security, says one of those experts, Philip Kegelmeyer, "it's networks you care about."

Kegelmeyer, who was principal investigator on a Sandia Laboratory Directed Research and Development Grand Challenge called Networks, says, "It's the rare bad person who operates alone. They need financing, have to wire money and rent, say, a truck.

"And if they want to infect your computer with malware, they can't just set up one server because some [defensive] network will figure it out and block it. Instead the bad guys set up a complicated web of servers. If one is blocked, the other takes over, so they've set up their own mini-networks. If you do the right science, you can detect the entire network — it's a network matching problem — and block access to it entirely."

Sandia provides tools for intelligence analysts to make those detections and connections. Kegelmeyer says the tools contain "lots of complex mathematics" that function in an almost epidemiological manner and work similarly to tracking the spread of a virus. "As in epidemiology," says Kegelmeyer, "sometimes what matters most is simply who you're spending time with. Our questions are, who did you interact with, who did you go bowling with and whose locations are linked to yours, so analysts can form a network of the closest links."

Intelligent maps

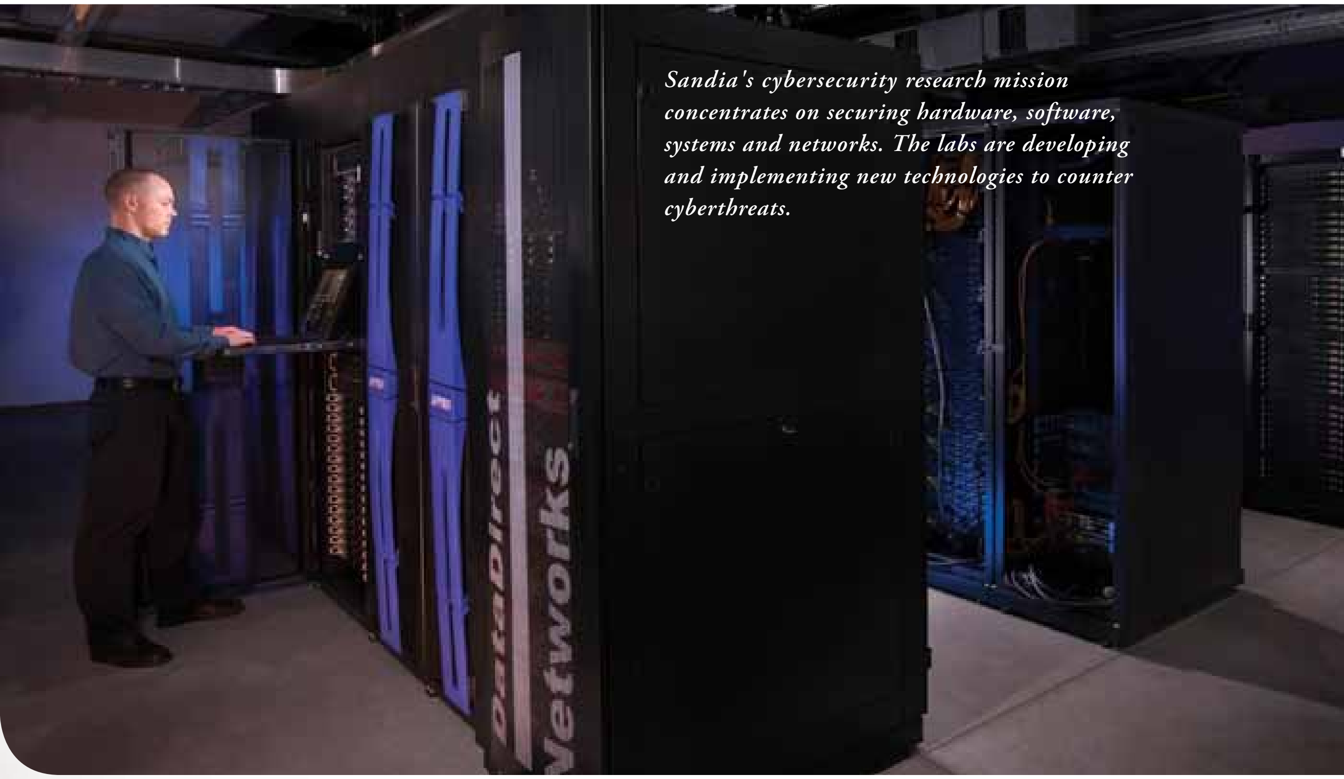
But that's only one way networks are of interest at Sandia.

In one grand challenge, researchers seek data networks that function as intelligent maps. These would offer solutions to analysts who otherwise would have to pore minutely over large areas.

Says senior manager Bruce Hendrickson, "Suppose we look at data on region X as observed by synthetic aperture radar and by satellites. We want to represent all this in a graph — a kind of map that shows buildings, railroad tracks and other physical features. We want to know how near they are to each other, their frequency of use and other factors.

to look for sites the analysts know are interesting. Say, in country X, we're looking for centrifuges. These would have to have a lot of electrical power, recent excavations and roads. So you would ask the computer whether it sees such collections of features in that country. Instead of the analyst looking everywhere, the analyst can query the computer's representation of that world.

"This is a very different way to think about imagery analysis, applying networks analytics, a much higher level of automation."



Sandia's cybersecurity research mission concentrates on securing hardware, software, systems and networks. The labs are developing and implementing new technologies to counter cyberthreats.

"So all these images are made available and there aren't enough skilled analysts to look at them, so the analysts pick the sites they think may be interesting to examine.

"But what if you could get a computer to look at them all and construct some representation of that world, some abstraction of its components, a linked network of all its features. Now an analyst tells the computer

Left: Sandia's Center for Cyber Defenders program trains students to protect and defend computer systems and networks from attack. The students help secure computers nationwide.

But what about abstract networks like Facebook, or the difficulty of modeling the changing number and locations of ships out at sea, or correlating the treatments of medical patients nationwide?

"Physical simulation has nice aspects to it because it represents the 3-D world, but in the abstract networks, you have huge complicated networks without geometric locality to them," Hendrickson says. In calculations of fluids, for example, an atom in one location affects the atoms immediately around it. "But in Facebook, it's hard to figure out how to use our traditional computers to show the closest links," he says. "If I wanted to see my relationship with Barack Obama, I'd have to look at all my friends and

Technician Armida Carbajal stays focused while tracking cyberthreats to Sandia Labs in the Cyber Engineering Research Laboratory.

their friends until I get to Barack Obama. In social networks, the first link might go to Kazakhstan."

Educating end-users

Beyond the problem of whether the computers of the future will have a single architecture that is all things

> *"...you come up with a solution and then the adversary figures out something else."*

to all people, there is still the issue of transmitting the information any of these computers produce to educate the humans using them.

"We [scientists] have blinders on. We think if we've solved a math problem, we're done," Hendrickson says. "But helping decision-makers is a matter of how information is represented, how it's communicated. These are huge issues in supporting people trying to make decisions."

Kegelmeyer offers a simple example. What's the best way, he asks, to call a doctor's attention to a suspected tumor in a mammograph — draw a circle around the suspected area or point a little red arrow at it?

"Intellectually, a circle or an arrow, it's the same thing," Kegelmeyer says. "Either points out the problem. But it turns out that which one is used is a big deal. Putting a circle around something has a containing effect on human psychology. It inadvertently lowers how much attention a doctor gives to examining the rest of the mammogram for problems the radiologist might not have noticed. That's a huge problem."

That's why Kegelmeyer pays attention to computer interfaces, because it's "so important to present information in the right way," he says. "Just giving humans better data doesn't mean they'll make better decisions."

To create the best interface, he says, "imagine you are trying to persuade someone of something. You think carefully about what they care about, what background they have, so you can customize your presentation to their perspective so they can understand it. That's what needs to be done in a computer interface."

Customization is easier said than done. "We all think we know how our brains work, so we think we understand how other brains work. So if it's good for me, it's good for you. But if you walk into someone else's computer, it's like walking into an alien brain. No one organizes like you do. It's hard to find a file, even though you know the file is there. People organize information differently. Our interfaces need to recognize that."

Psychological principles

While Apple can test its interface versions by paying many humans to see how quickly they can use technical features of a product, "they can do these expensive tests because they expect to make a ton of money selling iPhones," Kegelmeyer says. "Sandia doesn't work in volumes like that when it tests brand-new algorithms, so large-scale testing doesn't make sense."

Sandia must rely instead on basic psychological principles, like presenting mathematical quantities in ratios rather than percentages, which psychological tests have shown is easier for everyone to grasp.

Basic design guidelines say that people see color first and then shape, says Alisa Bandlow of Sandia's Operations Research and Knowledge Systems group. "We use color carefully so we don't accidentally highlight unimportant information." Grid lines, she says, should be thin, gray or a muted color, allowing the data to be the focus rather than the grid.

"Tomorrow's interfaces must pay more attention to the way humans perceive information," Kegelmeyer agrees.

In all these areas, Sandia has embraced the many problems of networking and interfacing, and with Laboratory Directed Research and Development and external funding is working on algorithms, architecture design and hardware layout as well as human psychology to come up with effective solutions.

"Some adversarial problems can never be totally solved," Kegelmeyer says, "because you come up with a solution and then the adversary figures out something else."

But a network of scientific superheroes can tackle a host of other issues and address today's most pressing social and defense challenges. ■

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LOOKING BACK

Red Storm was one of the most influential machines of its era. The Sandia-designed, Cray-built supercomputer left 124 descendants at 70 sites worldwide when it was turned off for good in mid-2012.

Red Storm broke new ground. It used off-the-shelf parts that made it cheaper to build, repair and upgrade. It was air-cooled instead of water-cooled so replacements and upgrades could be done while the machine was running. A custom-designed interconnect chip, operating system and software made the supercomputer remarkably efficient.

It was developed at Cray Inc. over 20 months instead of the usual five years. Sandia scientists traveled regularly to the company's Seattle, Wash., headquarters. From a peak speed of 41 teraflops in 2005, Red Storm was upgraded to 124 teraflops in 2006 and 284 teraflops in 2008.

Red Storm made possible innovative, highly sophisticated computer simulations to ensure the safety, security and reliability of the nuclear weapons stockpile. In 2008, a government satellite traveling more than 17,000 mph 153 miles above the Earth slipped out of orbit. The White House called, and Sandia used Red Storm full time for months to predict the outcome of complex destruction scenarios to help the USS Lake Erie safely shoot down the satellite with a rocket.

Cray CEO Pete Ungaro pays the supercomputer a huge compliment: "Virtually everything we do at Cray … comes from Red Storm."

— Neal Singer

Computer scientist Archie Gibson works inside the Red Storm supercomputer, an award-winning partnership between Cray Inc. and Sandia.